

# Simulation of X-ray Irradiation on Optics and Chamber Wall Materials for Inertial Fusion Energy

S. Reyes, J. F. Latkowski, R. P. Abbott, and W. Stein

**September 10, 2003** 

3<sup>rd</sup> International Conference on Inertial Fusion Science and Applications, Monterey, California, September 7-12, 2003

### **DISCLAIMER**

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.

This report has been reproduced directly from the best available copy.

Available electronically at <a href="http://www.doc.gov/bridge">http://www.doc.gov/bridge</a>

Available for a processing fee to U.S. Department of Energy
And its contractors in paper from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062

Telephone: (865) 576-8401 Facsimile: (865) 576-5728 E-mail: reports@adonis.osti.gov

Available for the sale to the public from U.S. Department of Commerce National Technical Information Service 5285 Port Royal Road Springfield, VA 22161 Telephone: (800) 553-6847

Facsimile: (703) 605-6900 E-mail: orders@ntis.fedworld.gov

Online ordering: <a href="http://www.ntis.gov/ordering.htm">http://www.ntis.gov/ordering.htm</a>

OR

Lawrence Livermore National Laboratory
Technical Information Department's Digital Library
http://www.llnl.gov/tid/Library.html

# SIMULATION OF X-RAY IRRADIATION ON OPTICS AND CHAMBER WALL MATERIALS FOR INERTIAL FUSION ENERGY

S. Reyes<sup>a</sup>, J. F. Latkowski, R. P. Abbott and W. Stein Lawrence Livermore National Laboratory, P. O. Box 808, L-641, Livermore, CA 94550 <sup>a</sup>Email: reyessuarez1@llnl.gov

### **ABSTRACT**

We have used the ABLATOR code to analyze the effect of the x-ray emission from direct drive targets on the optics and the first wall of a conceptual laser Inertial Fusion Energy (IFE) power plant. For this purpose, the ABLATOR code has been modified to incorporate the predicted x-ray spectrum from a generic direct drive target. We have also introduced elongation calculations in ABLATOR to predict the thermal stresses in the optic and first wall materials. These results have been validated with thermal diffusion calculations, using the LLNL heat transfer and dynamic structural finite element codes Topaz3d and Dyna3d. One of the most relevant upgrades performed in the ABLATOR code consists of the possibility to accommodate multi-material simulations. This new feature allows for a more realistic modeling of typical IFE optics and first wall materials, which may have a number of different layers.

Finally, we have used the XAPPER facility, at LLNL, to develop our predictive capability and validate the results. The ABLATOR code will be further modified, as necessary, to predict the effects of x-ray irradiation in both the IFE real case and our experiments on the XAPPER facility.

# I. INTRODUCTION

This paper describes the use of LLNL's ABLATOR code [1] as a predictive capability to assess the laser IFE chamber wall and final optics response to x-ray emission from direct drive targets. The ABLATOR ("Ablation By LAgrangian Transient One-dimensional Response") capability is a 1-D finite difference code for the calculation of material response to x-rays, which was originally developed to predict removal rates from the first wall and other components at the National Ignition Facility (NIF) in LLNL. Ablated chamber material is a major threat to the NIF laser final optics, as material condensing on these optics after a shot may cause damage with subsequent laser shots. The ABLATOR code uses an

explicit scheme for advancing in time. Four processes are included in the ablation model: energy deposition from the x-rays, transient thermal conduction, thermal expansion (which raises pressures and causes hydrodynamic motion), and removal of material through surface vaporization and various spall processes [1].

The main limitations of the use of ABLATOR for IFE are based on the lack of models for re-radiation and condensation, and the numerical stability of the code (the maximum time step size is limited by the typical stability conditions of the explicit method and other hydrodynamic stability requirements, such as maximum temperature change in a zone or surface vaporization rate). Also, the code only uses cold opacities, which means that the attenuation in a zone at a given photon energy stays constant throughout the run. However, if plasma is generated during x-ray deposition, the cold-opacity assumption would break down. Although this would be an issue in the case of liquid walls [2], it is not relevant in our case, as we are studying dry wall chambers or final optics from a laser IFE power plant design.

In the IFE case, we want to accurately predict the material removal from the chamber first wall and the laser final optics as a consequence of the target x-ray emission. The durability of these components is crucial for an attractive power plant design. Therefore, in this work we have modified the ABLATOR code and performed a series of calculations and validations in order to assess its suitability for IFE. The overall objective is to develop and experimentally benchmark a predictive capability, which can be used to analyze x-ray damage and/or ablation of IFE optical and chamber wall materials. While one can design components to avert single-shot melting and/or vaporization, little data are available for many-shot exposures at sub-threshold fluences. Similarly, only limited knowledge exists on the effects that impurities, contamination, surface rough surfaces. neutron/gamma-ray/ion irradiation have upon x-ray ablation. Through use of the x-ray irradiation facility XAPPER and further development of the ABLATOR code, our understanding of these areas will be advanced.

### II. ABLATOR MODIFICATIONS FOR IFE

We have updated and debugged the ABLATOR code in order to generate an enhanced version for use in IFE. The most relevant modifications include: implementation of direct and indirect drive x-ray spectra, ability to account for attenuation through a background gas, introduction of a restart capability, generation of a multimaterial version of the code, and addition of new materials (W, SiC and flibe) to the code's database. During the various steps of the upgrade process, we have also implemented various techniques to improve the code's numerical stability and debugged/tested the different modules.

We have used data from LASNEX calculations performed by J. Perkins at LLNL [3] to introduce the indirect and direct-drive target spectra for the bare target. In the case of direct drive, we have also implemented the escape spectrum after 6.5 Torr-cm of xenon gas, as well as the ability to attenuate IFE x-ray spectra out to distances of more than 6.5 m.

The restart capability allows the user to read in the temperature/enthalpy profile from a previous run as initial conditions for the current case. Figure 1 shows an example of this restart option used to model 3 consecutive pulses (IFE laser driver, prompt x-rays and secondary x-rays from direct drive target emissions) on an aluminum grazing incidence metal mirror (GIMM).

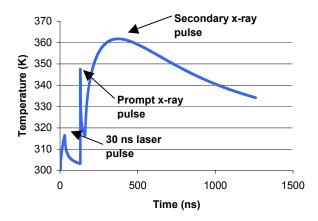


Figure 1. Simulation of laser pulse followed by prompt and secondary x-ray pulses from IFE target on an aluminum GIMM @ 85° and 30 m stand-off, protected by 10 mTorr Xe.

Laser IFE relevant materials have been added to the code's original database, such as tungsten and silicon carbide, and we have also collaborated with UCSD to add the molten salt flibe to the materials database, commonly used as liquid wall/coolant material in heavy-ion IFE conceptual designs.

For the materials investigated in the present work (aluminum and tungsten) we have also used the

temperature-dependant coefficient of thermal expansion to calculate elongation and therefore, predict the thermal stresses in the optic and first wall materials. Results of the stress calculations are compared to multiple cycle data of stress levels that lead to fatigue failure in the material. Allowable x-ray beam intensities can then be determined from calculated stress levels that do not exceed fatigue limits (when these are known). Calculations regarding thermal elongation and stress will be described in the results section.

Probably the most significant modification of this enhanced version of ABLATOR is the capability to perform multi-material simulations. This feature is essential for a realistic modeling of some IFE materials with multiple layers. This enhancement also turned out to be crucial for the accurate simulation of irradiation of Al/SiO<sub>2</sub> mirrors in the experimental facility XAPPER.

In order to validate the multi-material version of the ABLATOR, we developed the one dimensional heat transfer code RadHeat to determine temperature profiles in multi-layer components experiencing non-uniform volumetric heating from photon irradiation [4]. RadHeat is a C++ program that employs an explicit finite difference technique coupled with detailed material property files and user specified wall convection and emissivity boundary conditions. Samples can be composed of an arbitrary number of layers of any composition for which material files have been compiled and zone resolution within each layer is user specified. Benchmarks of the upgraded version of ABLATOR against RadHeat have yielded excellent agreement.

### III. RESULTS

As we noted previously, our goal is to develop a predictive capability for x-ray damage and/or ablation of IFE optical and chamber wall materials. In order to experimentally benchmark the ABLATOR calculations we have used the XAPPER x-ray irradiation facility in LLNL [5]. XAPPER is based upon a soft x-ray source designed and manufactured by PLEX LLC. A schematic of the typical facility layout is shown in Figure 2.

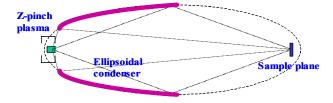


Figure 2. The plasma source and sample sit at the foci of an ellipsoid with a condensing optic between them.

The source is based upon a gas pinch that is currently operated with xenon discharges, although operation with

argon, nitrogen, and other gases is possible. Repetition rates of up to 10 Hz are supported. The experimental campaigns performed to-date in XAPPER have been limited to a fluence of ~0.2 J/cm². Whereas the original condensing optics suffered from a mid-frequency spatial roughness, it is expected that replacement optics will provide a focused EUV fluence over 1 J/cm². More details on the source's operation can be found in Refs. [5, 6]. The present work focuses on the two materials that have been irradiated so far in the facility: aluminum and tungsten. Aluminum is the leading material for the GIMMs final optics at a laser IFE power plant, whereas tungsten is considered to be a strong candidate for the laser IFE chamber first wall or armor.

### III.A. Aluminum Results

Regarding the irradiation of aluminum samples we have used the ABLATOR code to simulate two different types of experiments carried out at XAPPER.

First, we tried to replicate the results from a series of Al/SiO<sub>2</sub> mirrors exposures. The mirrors were irradiated at an x-ray fluence of 0.13-0.19 J/cm<sup>2</sup> for ~3000 pulses at a repetition rate of 8 Hz. As can be appreciated in Figure 3, significant surface damage was observed. A detailed description of the experimental campaigns at XAPPER is given in the paper by Latkowski et al. [5].

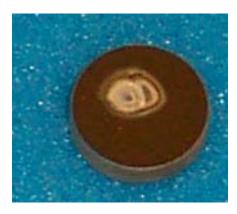


Figure 3. Photo of  $Al/SiO_2$  damaged mirror after ~6000 XAPPER pulses at 0.13 to 0.19 J/cm<sup>2</sup>. The two different spots correspond to two different runs with slightly different alignment of the focusing optic.

In order to verify if the damage was due to melting of the sample's surface, we performed a calculation using the multi-material version of the ABLATOR code. For this purpose we modeled considered a 100 nm layer of Al on top of a 3 mm SiO<sub>2</sub> substrate, and simulated irradiation with a single x-ray line at 113 eV (main emission line from Xe) assuming a fluence of 0.18 J/cm<sup>2</sup> for a pulse duration of 40 ns. Figure 4 shows the temperature evolution for the different zones of the model.

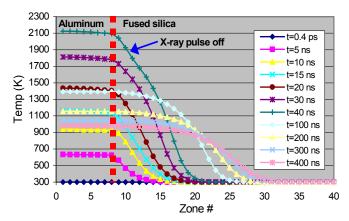


Figure 4. Temperature evolution in Al/SiO<sub>2</sub> ABLATOR simulation (first 7 zones constitute the thin Al layer, rest is SiO<sub>2</sub>).

It can be observed that the maximum surface tenperature is reached at the end of the 40 ns pulse, and that all the Al zones have reached a temperature above melting (933 K) at that point. Some of the front silica zones are also above the melting temperature for  $\rm SiO_2$  (1696 K). The prediction of surface damage through melting agrees with the effects observed after the irradiation of the samples in XAPPER.

Other than for predicting the damage on Al samples at XAPPER prototypical fluences, we have also used the ABLATOR code to simulate the temperature history of an IFE aluminum GIMM protected by 10 mTorr Xe, as a consequence of the direct drive target prompt x-ray emission. We have considered stand-off distances of 20 and 30 m. A maximum mirror length of 4 m from side to side was assumed in order to calculate the temperature gradient along the surface. Results are shown in Table I.

Table I. Temperature rise in the middle plane and at leading and far edges of an Al GIMM at 85° with 10 mTorr gas pressure.

Stand-off (m)	ΔT, mid (K)	∆T, lead (K)	∆T, far (K)	
20	109	137	89	
30	44	52	38	

We have used these data to calculate the XAPPER fluence that would be required to reach a similar  $\Delta T$  and temperature gradients along the mirror surface. The values in Table II indicate that the XAPPER fluences required are low enough to allow sample direct irradiation from the source with no need of the condensing optic that is usually part of the experimental layout (as long as the sample is positioned close enough to the source). The calculated stand-off distances from the x-ray source are only 6.5-10 cm. However, the removal of the ellipsoidal condenser, not needed in this case, would allow for free space in the surroundings of the source to the perform this type of in-situ optics testing.

Table II. XAPPER fluences and predicted temperature rise have been used to design an In-Situ Laser Diagnostic for IFE optics testing.

			Φ, far (J/cm2)		∆T, lead (K)	∆T, far (K)
6.5	5.92E-03	7.27E-03	4.91E-03	105	130	87
10	2.50E-03	2.85E-03	2.21E-03	45	49	39

The previous results have been used to design a special In-Situ Laser Diagnostic (ISLD). The ISLD is an optical apparatus used with XAPPER to study damage to aluminum mirrors in a pulsed X-ray environment comparable to that of a laser IFE fusion chamber. This is accomplished by using a low-power laser to probe an Xray exposed mirror in the XAPPER chamber. A schematic of the diagnostic system layout inside the XAPPER chamber can be seen in Figure 5. As damage to the exposed mirror accrues, the wavefront of the laser beam will become increasingly distorted giving qualitative and quantitative measures of the mirror damage process. By comparing the specific characteristics of a reference wavefront with those of a wavefront taken after some number of X-ray pulses, quantitative characterization of the damage process can be made.

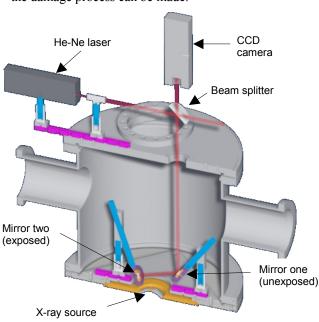


Figure 5. ISLD components and layout inside the XAPPER chamber.

# III. B. Tungsten Results

The XAPPER facility has also been used to study the effect of x-ray irradiation on tungsten. Samples of powder metallurgical tungsten, provided by the Oak Ridge National Laboratory, have been exposed to 0.18 J/cm<sup>2</sup> for 10,000 and 79,500 pulses. More detail on these

experiments is also described in Ref [5]. As opposed to the Al samples, no significant damage was noticeable by simple observation of the samples after irradiation. This agrees with the ABLATOR predictions, which indicate that the tungsten should remain under melting temperature ( $T_{melt} = 3695 \text{ K}$ ) for such fluence, as shown in Figure 6. This plot presents the ABLATOR results at the end of a XAPPER pulse (maximum surface temperature) for different x-ray fluences. It is expected that new optics will allow for fluences  $\sim 1 \text{ J/cm}^2$ . As can be observed in Figure 6, this fluence would be sufficient to melt tungsten.

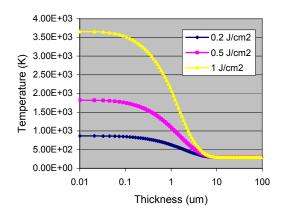


Figure 6. Temperature as a function of W sample thickness after a 40 ns long 113 eV x-ray pulse for x-ray fluences of 0.2, 0.5 and 1 J/cm<sup>2</sup>.

Although no damage was obvious after inspection of the samples at the microscope, detailed analysis through white-light interferometry of these and a control sample revealed local high-spots on the sample exposed to the most pulses. Such formations were not found on either the control sample or the one exposed to 10,000 pulses, so could be indicative of damage caused by rep-rated irradiation at sub-threshold temperatures. However, these results are considered preliminary, given that the spikes could be due to sample handling or to debris emitted from the plasma head. In the future, our samples will be mounted for less destructive handling, and anomalous spikes will be tested chemically in order to characterize the potential debris.

We have also used the multi-material version of the code to estimate the time-temperature history of an IFE wall consisting on a 50  $\mu$ m thick tungsten armor over a layer of 1 mm of ferritic steel. Figure 7 shows the temperature distribution at different times after the prompt x-ray pulse for this case and for a single tungsten layer.

The ABLATOR simulations described in this work only consider a single pulse, however, due to the cyclical nature of the beam, both in IFE and in the XAPPER facility, maximum fatigue stress limits need to be considered in determining allowable stresses in the material without failure occurring. For this purpose, the

thermal structural response of a tungsten wall due to an impinging x-ray beam was analytically investigated through thermal diffusion and dynamic structural calculations using the LLNL codes Topaz3d and Dyna3d [7, 8]. Simulations were performed for both a 40 nanoseconds XAPPER pulse at 0.08 J/cm<sup>2</sup> and for the IFE case (1 ns at 1 J/cm<sup>2</sup>). These calculations also were useful as benchmarking of ABLATOR's elongation module. ABLATOR's temperature and strain results were found to to be in good agreement with those from Topaz and Dyna. It was found that the peak stress in the XAPPER case was 80 ksi (corresponding to an x-ray energy flux of 0.08 J/cm<sup>2</sup>). Because 80 ksi is below the fatigue limit for W (98 ksi), the energy flux could be increased to 0.095 J/cm<sup>2</sup> with a peak temperature of 575 °C and a new fatigue stress of 95 ksi. The results for the IFE simulation showed compressive stresses ~5x larger, which would exceed the material strength.

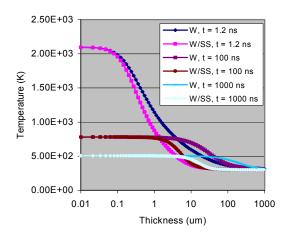


Figure 7. Temperature distribution at different times after the target prompt x-ray pulse, for a simple 1mm-thick W wall and for a SS409 wall coated with  $50 \mu m$  of W.

### IV. FUTURE WORK

We are in the process of developing and benchmarking a predictive capability for x-ray damage from IFE targets onto laser optics and chamber first walls. For that purpose, we have modified the code ABLATOR to better represent the phenomena due to IFE target x-rays and performed a series of calculations to study x-ray damage to two typical optic and chamber materials, aluminum and tungsten, respectively. In order to develop our methodology and validate the results we are using the XAPPER x-ray irradiation facility at LLNL.

An in-situ optics damage test has been planned in XAPPER that will help benchmark ABLATOR. This experiment will allow for advanced knowledge of Al GIMM optics under IFE conditions. Finally, a spectrometer was recently installed in the facility. This will allow us to implement the measured XAPPER x-ray spectrum into ABLATOR for more accurate predictions.

We will continue investigating the x-ray response of first wall material candidates. The installation of a new condensing optic (planned for September 2003) is expected to raise the XAPPER fluence to ~1 J/cm² so that IFE first wall conditions can be replicated in XAPPER. This will also allow for additional benchmarking and development of the ABLATOR code for its use as predictive capability for IFE x-ray damage.

# **ACKNOWLEDGMENTS**

Work performed under the auspices of the U. S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

# REFERENCES

- A. T. ANDERSON, A. K. BURNHAM, M. T. TOBIN, and P. F. PETERSON, "Modeling and Experiments of X-Ray Ablation of National Ignition Facility First Wall Materials," *Fusion Technol.* 30 (1996) 757-763.
- S. REYES, "ABLATOR Modeling of X-ray Effects on Liquid Walls," presented at the ARIES Liquid Wall Dynamics Town Meeting, Livermore, CA, May 2003
- L. J. PERKINS, M. TABAK, R. BETTI, A. SCHMITT, and S. OBENSCHAIN, "High-Yield, Direct-Drive Targets for Inertial Fusion Energy," Presented at the Third International Conf. on Inertial Fusion Sciences and Applications, Monterey, CA, Sep. 7-12, 2003.
- 4. R. P. ABBOTT, "RadHeat V\_1.1a Benchmarks," to be published as LLNL report, 2003.
- J. F. LATKOWSKI et al., "Rep-Rated X-Ray Damage and Ablation Experiments for IFE and ICF Applications," presented at the Third International Conf. on Inertial Fusion Sciences and Applications, Monterey, CA, Sept 7-12, 2003.
- 6. M. McGEOCH, "Radio-Frequency-Preionized Xenon Z-Pinch Source for Extreme Ultraviolet Lithography," *Appl. Optics* **37** (1998) 1651-1658.
- 7. A. B. SHAPIRO, "TOPAZ3D Users Manual— A 3-dimensional Finite Element Heat Transfer Code", Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MA-140137, May 2000.
- 8. R. G. WHIRLEY, B. E. ENGELMANN, "DYNA2D, A Nonlinear, Explicit, Two Dimensional Finite Element Code For Solid Mechanics, User Manual", Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MA-110630, April 1992.